

	Type	Hits	Search Text	DBs	Time Stamp	Comments
1	BRS	29	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 with chemical with compound\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 12:57	
2	BRS	18	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 with chemical with compound\$1 and chemical\$2 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 13:07	
3	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 with chemical with compound\$1 and chemical\$2 with molecule\$1 same solid with (state\$1 or status or condition\$1)	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 13:08	
4	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 same solid with (state\$1 or status or condition\$1)	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 15:50	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
5	BRS	44	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 and solid with (state\$1 or status or condition\$1)	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 15:50	
6	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 and solid with (state\$1 or status or condition\$1) and energ\$3 with pack\$3 with interact\$3 same parameter\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 15:51	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
7	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 and solid with (state\$1 or status or condition\$1) and energ\$3 with pack\$3 with interact\$3	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 15:52	
8	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 and solid with (state\$1 or status or condition\$1) and energ\$3 with pack\$3 with (interface or interact\$3) same parameter\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:08	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
9	BRS	11	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 and solid with (state\$1 or status or condition\$1) and energ\$3 same parameter\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:13	
10	BRS	4	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 and solid with (state\$1 or status or condition\$1) and energ\$3 same pack\$3 same parameter\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:13	
11	BRS	4	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 with chemical with compound\$1 and chemical\$2 with molecule\$1 and (solid- dtate or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:14	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
12	BRS	4	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 and (solid- dtate or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:15	
13	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 and model\$1 with (solid-dtate or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:14	
14	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical with compound\$1 and chemical\$2 with molecule\$1 and model\$1 with (solid-dtate or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:24	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
15	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and chemical\$2 with molecule\$1 and model\$1 with (solid-dtate or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:28	
16	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and chemical\$2 with molecule\$1 and model\$1 with (solid-state or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:29	
17	BRS	3	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and chemical\$2 with molecule\$1 and model\$1 same (solid-state or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:29	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
18	BRS	3	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3), with solubil\$5 and chemical\$2 with compound\$1 and model\$1 same (solid- state or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:29	
19	BRS	7	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and (solid-state or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:30	
20	BRS	58	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and model\$1 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:32	
21	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and solid with model\$1 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:13	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
22	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and solid same model\$1 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:13	
23	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and assembl\$3 with cluster\$1 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:14	
24	BRS	10	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and cluster\$1 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:29	
25	BRS	6	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and build\$3 with model\$1 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:29	



	Type	Hits	Search Text	DBs	Time Stamp	Comments
26	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and build\$3 with model\$1 with molecule\$1 with cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:33	
27	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and model\$1 with molecule\$1 with cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:33	
28	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 with molecule\$1 and chemical\$2 with compound\$1 and state with model\$1 with cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:44	
29	BRS	4	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 with molecule\$1 and chemical\$2 with compound\$1 and cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:45	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
30	BRS	6	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solub\$7 with molecule\$1 and chemical\$2 with compound\$1 and cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:48	
31	BRS	1122	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1 and cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:49	
32	BRS	402	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1 and (database\$1 or librar\$3 or profile\$1) with chemical\$2 with molecule\$1 and cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:49	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
33	BRS	98	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1 and (database\$1 or librar\$3 or profile\$1) with chemical\$2 with molecule\$1 and cluster\$1 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:58	
34	BRS	6	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1 and (database\$1 or librar\$3 or profile\$1) with chemical\$2 with molecule\$1 and cluster\$1 with molecule\$1 and energ\$3 with parameter\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:58	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
35	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1 and (database\$1 or librar\$3 or profile\$1) with chemical\$2 with molecule\$1 and cluster\$1 with molecule\$1 and quantit\$5 with parameter\$1 with descriptor\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 11:06	
36	BRS	4	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1 and (database\$1 or librar\$3 or profile\$1) with chemical\$2 with molecule\$1 and cluster\$1 with molecule\$1 and energ\$3 with pack\$3	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 11:06	
37	BRS	2604	702/22,30,31,32,179,183.cc 1s.	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 12:56	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
38	BRS	30	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 with chemical with compound\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 12:56	
39	BRS	19	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 with chemical with compound\$1 and chemical\$2 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 12:57	
40	BRS	8	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 with chemical with compound\$1 and (identify\$3 or determin\$3 or detect\$3) with chemical\$2 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 13:00	
41	BRS	37	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and (identify\$3 or determin\$3 or detect\$3) with chemical\$2 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 13:00	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
42	BRS	14	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and (identify\$3 or determin\$3 or detect\$3) with chemical\$2 with molecule\$1 and solid with (state\$1 or condition\$1 or status)	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 13:01	
43	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and (identify\$3 or determin\$3 or detect\$3) with chemical\$2 with molecule\$1 and solid with (state\$1 or condition\$1 or status) and assembl\$3 with cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 13:02	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
44	BRS	9	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and (identify\$3 or determin\$3 or detect\$3) with chemical\$2 with molecule\$1 and solid with (state\$1 or condition\$1 or status) and cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 13:05	
45	BRS	0	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and (identify\$3 or determin\$3 or detect\$3) with chemical\$2 with molecule\$1 and scomput\$7 with model\$1 and cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 13:05	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
46	BRS	11	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and (identify\$3 or determin\$3 or detect\$3) with chemical\$2 with molecule\$1 and comput\$7 with model\$1 and cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 13:05	
47	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 with chemical with compound\$1 and chemical\$2 with molecule\$1 same solid with (state\$1 or status or condition\$1)	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 13:08	
48	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 same solid with (state\$1 or status or condition\$1)	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 15:50	



	Type	Hits	Search Text	DBs	Time Stamp	Comments
49	BRS	45	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 and solid with (state\$1 or status or condition\$1)	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 15:50	
50	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 and solid with (state\$1 or status or condition\$1) and energy with pack\$3 with interact\$3 with parameter\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 15:51	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
51	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 and solid with (state\$1 or status or condition\$1) and energ\$3 with pack\$3 with interact\$3	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 15:52	
52	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 and solid with (state\$1 or status or condition\$1) and energ\$3 with pack\$3 with (interface or interact\$3) same parameter\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:08	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
53	BRS	11	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 and solid with (state\$1 or status or condition\$1) and energ\$3 same parameter\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:13	
54	BRS	4	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 and solid with (state\$1 or status or condition\$1) and energ\$3 same pack\$3 same parameter\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:13	
55	BRS	4	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 with chemical with compound\$1 and chemical\$2 with molecule\$1 and (solid- dtate or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:13	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
56	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 and model\$1 with (solid-dtate or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:14	
57	BRS	4	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 with chemical with compound\$1 and chemical\$2 with molecule\$1 and (solid- dtate or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:15	
58	BRS	4	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubilit\$3 and chemical with compound\$1 and chemical\$2 with molecule\$1 and (solid- dtate or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:15	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
59	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical with compound\$1 and chemical\$2 with molecule\$1 and model\$1 with (solid-dtate or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:24	
60	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and chemical\$2 with molecule\$1 and model\$1 with (solid-dtate or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:29	
61	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and chemical\$2 with molecule\$1 and model\$1 with (solid-state or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:29	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
62	BRS	3	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and chemical\$2 with molecule\$1 and model\$1 same (solid-state or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:29	
63	BRS	3	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and model\$1 same (solid- state or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:29	
64	BRS	7	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and (solid-state or solid with state\$1) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:30	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
65	BRS	64	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and model\$1 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/04 16:32	
66	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and solid with model\$1 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:13	
67	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and solid same model\$1 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:13	
68	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and assembl\$3 with cluster\$1 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:21	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
69	BRS	10	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and cluster\$1 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:29	
70	BRS	6	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and build\$3 with model\$1 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:29	
71	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and build\$3 with model\$1 with molecule\$1 with cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:33	
72	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 and chemical\$2 with compound\$1 and model\$1 with molecule\$1 with cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:33	



	Type	Hits	Search Text	DBs	Time Stamp	Comments
73	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 with molecule\$1 and chemical\$2 with compound\$1 and state with model\$1 with cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:44	
74	BRS	4	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solubil\$5 with molecule\$1 and chemical\$2 with compound\$1 and cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:45	
75	BRS	7	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with solub\$7 with molecule\$1 and chemical\$2 with compound\$1 and cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:48	
76	BRS	1206	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1 and cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:49	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
77	BRS	442	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1 and (database\$1 or librar\$3 or profile\$1) with chemical\$2 with molecule\$1 and cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:49	
78	BRS	108	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1 and (database\$1 or librar\$3 or profile\$1) with chemical\$2 with molecule\$1 and cluster\$1 with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:58	
79	BRS	6	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1 and (database\$1 or librar\$3 or profile\$1) with chemical\$2 with molecule\$1 and cluster\$1 with molecule\$1 and energ\$3 with parameter\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 10:58	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
80	BRS	2	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1 and (database\$1 or librar\$3 or profile\$1) with chemical\$2 with molecule\$1 and cluster\$1 with molecule\$1 and quantit\$5 with parameter\$1 with descriptor\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 11:06	
81	BRS	4	(predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1 and (database\$1 or librar\$3 or profile\$1) with chemical\$2 with molecule\$1 and cluster\$1 with molecule\$1 and energ\$3 with pack\$3	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 11:06	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
82	BRS	76	(702/22,30,31,32,179,183.c cls.) and (predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 13:28	
83	BRS	51	(702/22,30,31,32,179,183.c cls.) and (predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 13:29	
84	BRS	27	(702/22,30,31,32,179,183.c cls.) and (predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1 and cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 13:28	

	Type	Hits	Search Text	DBs	Time Stamp	Comments
85	BRS	17	(702/22,30,31,32,179,183.c cls.) and (predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1 and (database\$1 or librar\$3 or profile\$1) with chemical\$2 same molecule\$1 and cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 13:29	
86	BRS	13	(702/22,30,31,32,179,183.c cls.) and (predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1 and (database\$1 or librar\$3 or profile\$1) with chemical\$2 with molecule\$1 and cluster\$1	US-PGPUB; USPAT; EPO; JPO; DERWENT; IBM_TDB	2006/05/05 13:29	
87	BRS	26	(702/22,30,31,32,179,183.c cls.) and (predict\$3 or estimat\$3 or validat\$3 or evalidat\$3) with molecule\$1 and chemical\$2 with compound\$1	US-PGPUB	2006/05/05 13:30	

	U	1	Document ID	Issue Date	Pages	Title	Current OR	Current XRef	Retrieval Classif
1			US 2005028332 0 A1	20051222	31	Method and system for profiling biological systems	702/22		702/22
2	X		US 2005027327 5 A1	20051208		Method and system for profiling biological systems	702/22		702/22
3	X		US 2005022859 2 A1	20051013		Method and device for partitioning a molecule	702/19	702/22	702/22
4	X		US 2005020978 8 A1	20050922		Method and system of computing and rendering the nature of the chemical bond of hydrogen-type molecules and molecular ions	702/22		702/22
5	X		US 2005013645 0 A1	20050623		Pharmacophore model generation and use	435/6	702/19; 702/22	702/22

	U	I	Document ID	Issue Date	Pages	Title	Current OR	Current XRef	Retrieval Classif
6	X		US 2005011983 5 A1	20050602		Method and apparatus for analysis of molecular combination based on computational estimation of electrostatic affinity using basis expansions	702/19	345/501; 702/22	702/22
7	X		US 2005011983 4 A1	20050602		Method and apparatus for analysis of molecular combination based on computations of shape complementarity using basis expansions	702/19	345/501; 702/22	702/22
8	X		US 2005010057 5 A1	20050512		Arthropod repellent pharmacophore models, compounds identified as fitting the pharmacophore models, and methods of making and using thereof	424/405	702/19; 702/22	702/22

	U	1	Document ID	Issue Date	Pages	Title	Current OR	Current XRef	Retrieval Classif
9	X		US 2005009685 2 A1	20050505		Method for increasing the stability and intensity of odorant molecules	702/22	424/401	702/22
10	X		US 2004022545 1 A1	20041111	8	Method of prediction of solubility of chemical compounds	702/22		702/22
11	X		US 2004021039 6 A1	20041021		METHODS AND STRUCTURE FOR AUTOMATED ACTIVE PHARMACEUTICALS DEVELOPMENT	702/19	702/22; 705/1	702/22
12	X		US 2004012148 7 A1	20040624		Method for enhanced accuracy in predicting peptides using liquid separations or chromatography	436/514	702/19; 702/22	702/22
13	X		US 2004011712 5 A1	20040617		Drug discovery method and apparatus	702/19	702/22	702/22
14	X		US 2004010705 4 A1	20040603		Method for determining discrete quantitative structure activity relationships	702/19	702/22	702/22



	U	1	Document ID	Issue Date	Pages	Title	Current OR	Current XRef	Retrieval Classif
15	X		US 2004003447 7 A1	20040219		Methods for modeling chromatographic variables	702/19	702/22	702/22
16	X		US 2004001529 9 A1	20040122		Clustering conformational variants of molecules and methods of use thereof	702/19	702/22	702/22
17	X		US 2004001413 7 A1	20040122		Method for producing and screening mass-coded combinatorial libraries for drug discovery and target validation	435/7.1	436/518; 702/22	702/22
18	X		US 2003016713 5 A1	20030904		Non-linear modelling of biological activity of chemical compounds	702/22		702/22
19	X		US 2003011499 1 A1	20030619		Prediction of molecular polar surface area and bioabsorption	702/22		702/22

	U	1	Document ID	Issue Date	Pages	Title	Current OR	Current XRef	Retrieval Classif
20	X		US 2003011499 0 A1	20030619		Prediction of molecular polar surface area and bioabsorption	702/19	702/22; 703/11; 703/12	702/22
21	X		US 2003010047 5 A1	20030529	35	Predicting taxonomic classification of drug targets	514/1	702/19; 702/22	702/22
22	X		US 2003002833 0 A1	20030206	24	System and method for aqueous solubility prediction	702/30	702/31	702/30; 702/31
23	X		US 2002016152 8 A1	20021031		Tool for lipophilicity determination in drug discovery basic and neutral compounds	702/22		702/22
24	X		US 2002001366 2 A1	20020131		PHARMACOKINETIC-BASED DRUG DESIGN TOOL AND METHOD	702/19	435/283.1 ; 435/287.1 ; 702/22	702/22
25	X		US 2002001055 0 A1	20020124		PHARMACOKINETIC-BASED DRUG DESIGN TOOL AND METHOD	702/19	435/283.1 ; 435/287.1 ; 702/22	702/22

	U	1	Document ID	Issue Date	Pages	Title	Current OR	Current XRef	Retrieval Classif
26	X		US 2001004196 4 A1	20011115		PHARMACOKINETIC-BASED DRUG DESIGN TOOL AND METHOD	702/19	422/68.1; 702/22	702/22